Feldbacher, Held, and Assaad Reply: Recently, we introduced a projective quantum Monte Carlo (PQMC) algorithm for simulating the Anderson impurity model (AIM) [1]. The preceding critique [2] based on the orthogonality catastrophe (OC) [3] is invalid: (i) There is no OC in [1], and it is generally not "unpractical" to avoid it. (ii) The OC does not affect our results.

Concerning (i): The OC theorem [3] states: If a Hamiltonian H_T is perturbed by a local disorder potential and/or interaction H' to a Hamiltonian $H = H_T + H'$, the overlap of the ground states of H and H_T is

$$|\langle\psi_G|\psi_T\rangle| \sim N^{-\alpha}, N \text{being the numer of bath sites.} \quad (1)$$

What Katsnelson [2] overlooked is that $\alpha = 0$ in [1]. The α of Eq. (1) is given by the difference between the scattering phase for H_T and H (φ_T and φ_G, respectively), i.e., $\alpha \sim (\varphi_T - \varphi_G)^2$[4]. According to the Friedel sum rule, the scattering phase φ is related to the average number of electrons on the impurity site: $\varphi = \pi/2\ n_d$. Since n_d is the same for H and H', we have $\varphi_T = \varphi_G$, and hence $\alpha = 0$. There is no OC.

Note that our calculations in [1, 5] are for half-filled bands, so that we automatically have $\alpha = 0$. But also off half-filling one is free to choose a H_T with the same n_d.

This proof based on Friedel's sum rule has been incorporated in [2], where it is now argued that using a H_T without OC is "unpractical" [2] because one would need an (analytically) "exact answer for n_d" [2]. We reject this critique. For a *numerical* algorithm, it is perfectly legitimate to calculate n_d *numerically*. We have done so in practice [6].

Concerning (ii): The OC is irrelevant for our calculations since for long enough projection time θ we obtain the same Green function $G(\tau)$ with and without OC, see Fig. 1. The calculations of Fig. 1 have been done for an AIM with on-site hybridization $V = 1$, a constant bath density of states ranging from -1 to 1 (with $N \to \infty$ bath sites), imaginary time discretization $\Delta\tau = 0.1$, impurity level $\epsilon_d = 0.5$, and Coulomb interaction $U = 0$ (for maximizing precision). The trial AIM with OC was half-filled, i.e., $\epsilon_d^{\text{trial}} = 0$, $n_d^{\text{trial}} = 1$ instead of $\epsilon_d = 0.5$, $n_d \sim 0.7$. For long enough projection θ, the Green function with OC converges to the exact result. At $\theta = 100$ (250), the average difference to the exact $G(\tau)$ is already as small as $7 \cdot 10^{-4}$ ($3 \cdot 10^{-4}$). Also, $n_d = 2[1 - G(\tau = 0)]$ is obtained extremely precisely even with OC.

Technically, one can understand the irrelevance of the OC by considering that we have integrated out the N bath sites of Eq. (1) [1, 7]. The algorithm is exactly the same with OC ($N \to \infty$) and without OC (finite N). For large enough but finite N, also the non-interacting input Green function can be the same as for $N \to \infty$, within any given accuracy. Hence, the results are the same with and without OC.

Physically, one can understand the irrelevance of the OC by considering that the OC theorem [3] holds in the

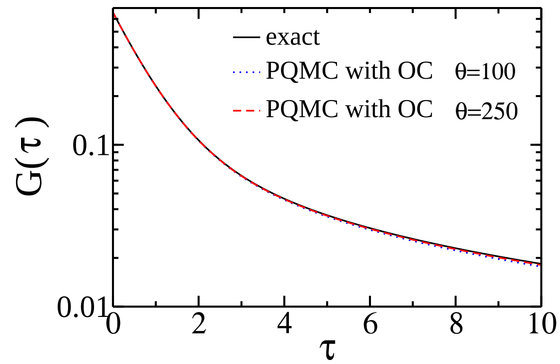

FIG. 1: (Color online) PQMC Green function with OC and without OC (exact). For long enough projection θ, the Green function with OC converges to the exact result. Note the logarithmic scale of the y axis.

metallic, (quasi-)particle regime and only for $N \to \infty$. Then, however, the ground state and excited states with a finite number of particle-hole excitations, have the same physical properties, since the finite number of particle-hole excitations becomes irrelevant for $N \to \infty$. Ground state and such low-lying excited states yield the same equilibrium (ground state) Green function [8]. This explains, why we obtain the correct results, e.g., in Fig. 1, even with OC. The OC is irrelevant for our calculations. Katsnelson's objection [2] is not valid.

M. Feldbacher[1], K. Held[1], and F. F. Assaad[2]

[1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany

[2] Institut für theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

Received
DOI:
PACS numbers:

[1] M. Feldbacher, K. Held, and F. F. Assaad, Phys. Rev. Lett. **93**, 136405 (2004).
[2] M. I. Katsnelson, preceding comment.
[3] P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967); Phys. Rev. **164**, 352 (1967).
[4] See, e.g., K. Yamada and K. Yosida, Progr. Theor. Phys. **60**, 353 (1978).
[5] R. Arita and K. Held, Phys. Rev. B **72**, 201102 (2005).
[6] R. Arita and K. Held, Phys. Rev. B **73**, 064515 (2006).
[7] J. E. Hirsch and R. M. Fye, Phys. Rev. Lett. **56**, 2521 (1986).
[8] Also note O. Gunnarsson and K. Schönhammer, Phys. Rev. B **26**, 2765 (1982), where—for the original OC model of non-interacting electrons [3]—it was proved that the ground state and the lowest excited states (even with infinitely many particle-hole excitations, less then $\sim N^{1/2}$) yield the same local expectation values for equal-time one-particle operators in the limit $N \to \infty$.